REPORT DOCUMENTATION PAGE

AFRL-SR-BL-TR-00-

0215

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	4/15/00	Final Technical Report ... 2/14/00

4. TITLE AND SUBTITLE

(U) Evaluation of Closure Models of Turbulent Diffusion Flames

5. FUNDING NUMBERS

PE - 61102F
PR - 2308
SA - BS
G - F49620-97-1-0092

6. AUTHOR(S)

G. Kosály and J. J. Riley

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Dept. of Mechanical Engineering
Box 352600, University of Washington
Seattle, WA 98195-2600

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

AFOSR/NA
110 Duncan Avenue, Suite B115
Bolling AFB DC 20332-0001

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

20000614 080

12a. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

Modeling methods applied in the field of turbulent combustion were investigated via Direct Numerical Simulations (DNS) and theoretical analysis with an emphasis on subgrid-scale modeling to be applied in Large Eddy Simulations (LES). The DNS results supported the conditional moment closure approximation, refuted the common modeling of differential diffusion effects, raised a suggestion for valid modeling of differential diffusion, resolved outstanding theoretical issues regarding mixing layers, and demonstrated the need for including flamelet/flamelet interactions in the modeling of extinction/reignition events. The DNS methodology was reconfirmed by comparison to the classical laboratory results of Comte-Bellot and Corrsin. A new subgrid-scale model (Large Eddy Laminar Flamelet; LELFM, a quasi-steady model) was established and applied to the prediction of laboratory results in a simulated mixing layer with nitric oxide/ozone reaction. The results support the modeling. New results were derived and confirmed via DNS regarding the the subgrid-scale modeling of the filtered mixture fraction, its second moment and dissipation rate.

14. SUBJECT TERMS	15. NUMBER OF PAGES
	8
	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	UL

NSN 7540-01-280-5500

Standard Form 298 (890104 Draft)
Prescribed by ANSI Std. 239-18
298-01

EVALUATION OF CLOSURE MODELS OF TURBULENT DIFFUSION FLAMES

(AFOSR Grant No. F49620-1-0092)

Principal Investigators: George Kosály and J. J. Riley
Department of Mechanical Engineering
University of Washington, Seattle, WA, 98195-2600

DISCUSSION OF RESEARCH PROGRESS

(February 15, 1977- February 15, 2000)

This review is primarily based on papers that have been published in the archival literature.

Direct Numerical Simulation Investigations

Our group performed a systematic study of the applicability of the Conditional Moment Closure (CMC) approximation that has been introduced by Bilger (1993). The work started before the time period covered by this report with the investigations of Mell et al. (1994), who used a one-step chemistry approach, and Montgomery et al. (1993) who applied more realistic, hydrogen/oxygen chemistry. Both investigations considered incompressible flow conditions. The new work of Montgomery et al. (1997) presents three-dimensional direct numerical simulations of a seven-species, ten-reaction hydrogen-oxygen mechanism in decaying, variable density, isotropic turbulence.

An obvious limitation on the CMC approach is the influence of high activation energy on the negligibility of the conditional fluctuations. Accordingly, one of the focuses of Montgomery has been the investigation of the H+O2<-->OH+O reaction. The detailed study has fully corroborated the validity of the CMC approach to predict the DNS data. The DNS data were also used to check the validity of the steady-state approaximation to predict O and OH and to investigate the applicability the manifold-approach of Maas and Pope (1994).

Differential diffusion is due to differences in the molecular diffusivities of different species, momentum and heat. Of special interest to the modeling of hydrogen and hydrocarbon flames is the influence of the preferential diffusion of H_2 and H. We have investigated the problem of differential diffusion via DNS and theoretical derivations in two consecutive papers (Nilsen et al., 1997, 1999).

The first paper studies the influence of differential diffusion on mixing; the second paper uses the results of the investigation of mixing in reacting cases. The simulations show that the effects of differential diffusion disappear with increasing values of the Reynolds and Peclet numbers. This is in line with theoretical expectations and points to the erroneous nature of the modeling commonly used (Pitsch and Peters, 1998). It is shown furthermore that the clue to the modeling of the influence of differential diffusion is in the modeling of the conditional fluctuations. Whereas limitations on the resolution did not allow to investigate the modeling in detail, looking at our results in conjunction with similar results of Kronenburg and Bilger (1998), a two-step procedure can be established to predict differential diffusion effects, e.g., in a hydrogen-air flame. In the first step differential diffusion effects are neglected and the conditionally averaged specie mass fractions are computed. In the second step we use the conditional averages calculated in the first step and numerical constants determined from DNS to model the conditional averages in the equations of H_2 and H and solve the equations again. Since differential diffusion is related to the small scales whose dynamics is approximately universal, the parameter values obtained from DNS are expected to be applicable in both RANS and LES.

Recent (yet unpublished) DNS results investigate the influence of the local value of the scalar dissipation rate on the extinction-reignition of "flamelets". The results demonstrate that quasisteady-flamelet ideas can be used to predict extinction but are insufficient to describe the process of reignition. The reason for this is that present day flamelet modeling is based on the concept of independent "counterflow-flamelets", whereas reignition is most of the time not autoignition but is promoted by neighboring hot flamelets. We are presently in the process of generalizing the flamelet model by introducing interaction between the flamelets.

Subgrid-Scale Modeling

We have developed one of the first subgrid-scale models for (LELFM) use in large-eddy simulations of turbulent reacting flows (Cook and Riley, 1994, 1997; Cook, Riley and Kosaly, 1997). This model, utilizing flamelet concepts combined with some of the latest features of subgrid-scale modeling, addresses non-premixed, continuously burning reactions at somewhat high Damkohler numbers. It has relatively low computational overhead associated with the chemistry modeling, and can be applied to realistic thermo-chemistry, giving it a broad range of applicability. A number of researchers are now working on related subgrid-scale modeling approaches.

Our principal idea is to use the quasi-steady flamelet (LELFM) approximation in the subgrid-scale modeling of turbulent flames that are burning far from extinction. Cha and Kosaly (2000) published a new investigation of the validity condition of quasi-steady flamelet modeling. The condition given deviates from the condition commonly used (Peters, 1999). The new condition accounts for the somewhat counterintuitive finding that the quasi-steady approximation works better close to nozzle in a jet flame than close to the tip. (Note that, close to the tip, the approximation is not needed since the quasi-steady flamelet model can be replaced by the equilibrium chemistry approach.) The theoretical derivation is supplemented by computed (RANS) results referring to a hydrogen/air jet flame.

More recently we have been examining various assumptions in the subgrid model by comparisons of modeling predictions mainly with results from high resolution, direct numerical simulations. Specifically we have addressed the subgrid-scale modeling of the filtered mixture fraction, its second moment, and its dissipation rate (de Bruyn Kops et al., 1998), quantities which are called for in the subgrid-scale modeling procedure. To test the model further, we have recently performed very high resolution direct numerical simulations of the nitric oxide/ozone experiments of Bilger et al. (1991) (de Bruyn Kops, 1999; de Bruyn Kops and Riley, 2000b); the results are being used for further validation of the subgrid-scale model. The general result of our validation studies to date is that the model works very well for the range of problems that it was intended, i.e., continuous burning, non-premixed, somewhat high Damkohler number cases.

Considerable effort has been made in improving and expanding the methodology of direct numerical and large-eddy simulation of reacting flows, in order to utilize the simulations to better understand the combusting flows and also to test models for RANS and large-eddy simulations. With a detailed understanding of the methodology and the efficient use of DOD high performance computers, we were the first to perform accurate direct numerical simulations of the classic laboratory experiments of Comte-Bellot and Corrsin (1971) (de Bruyn Kops and Riley, 1998). This has been followed by the first accurate direct numerical simulations of turbulent scalar mixing layers, and the resolution of some outstanding theoretical issues related to mixing (de Bruyn Kops and Riley, 2000a). In both cases the agreement with the laboratory data was very good, giving confidence in the methodology. Accurate simulations of both of these cases were required in order to simulate the experiments of Bilger et al.,

which addressed the same flow and mixing configuration. Recently the direct numerical simulation methodology was extended to very accurate simulations of strongly temperature-dependent reactions (de Bruyn Kops, 1999; de Bruyn Kops and Riley, 2000), which is now being used in our studies of extinction and re-ignition. Finally, at the present we are developing the methodology for very accurate direct numerical and large-eddy simulations of reacting turbulent jets, both for model testing and for comparisons with laboratory data.

References

Bilger, R. W., L. R. Saetran, and L. V. Krishnamoorthy, "Reaction in a scalar mixing layer", *J. Fluid Mech.*, Vol. 233, p. 211, 1991.

Bilger, R. W., "Conditional moment closure for turbulent reacting flow", *Phys. Fluids A*, Vol. 5, p. 436, 1993.

Cha M. Chong and G. Kosaly, "Quasi-Steady Modeling of Turbulent Nonpremixed Combustion", Accepted for publication by Comb. Flame, 2000. N. Peters, "Turbulent Combustion", Manuscript sent to Cambridge University Press, 1999.

Comte-Bellot, G., and S. Corrsin, "Simple Eulerian time correlation of full and narrow-band velocity signals in grid-turbulence", *J. Fluid Mech.*, Vol. 48, p. 273, 1971.

Cook, A. W., and Riley, J. J., "A subgrid model for equilibrium chemistry in turbulent flows", *Phys. Fl.*, Vol. 6(8), pp. 2868-2870, 1994.

Cook, A. W., and J. J. Riley, "Subgrid-scale modeiing for turbulent, reacting flows", *Comb. Flame*, Vol. 109, pp. 439-448, 1997.

Cook, A. W., J. J. Riley, and G. Kosaly, "A laminar flamelet approach to subgrid-scale chemistry in turbulent flows", *Comb. Flame*, Vol. 109, pp. 332-341, 1997.

de Bruyn Kops, S. M. "Large-Eddy Simulation of Non-Premixed Turbulent Combustion", Ph.D. thesis, University of Washington, 1999.

de Bruyn Kops, S. M., and J. J. Riley, "Direct numerical simulation of laboratory experiments in isotropic turbulence", *Phys. Fluids*, Vol. 10, pp. 2125-2127, 1998.

de Bruyn Kops, S. M., and J. J. Riley, "Re-examining the thermal mixing layer with numerical simulations", *Phys. Fluids*, Vol. 12(1), pp. 185-192, 2000a.

de Bruyn Kops, S.M., and J. J. Riley, (2000)"Mixing Models for Large-eddy Simulation of Non-premixed Turbulent Combustion" , *Journal of Fluid Engineering,* Submitted for publication, 2000b.

de Bruyn Kops, S. M., J. J. Riley, G. Kosaly and A. W. Cook, "Investigation of modeling for non-premixed turbulent combustion", *Flow, Turb. and Comb.*, Vol. 60, pp. 105-122, 1998.

Kronenburg and Bilger (1998) ,personal communication

Maas, U. and Pope, S. B., Twenty-Fifth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, 1994, pp. 1349-1356.

Mell, W. E., Nilsen, V., Kosaly, G., and Riley, J. J., "Investigation of closure models of nonpremixed turbulent reacting flows", *Phys. Fluids A*, Vol. 6(3), pp. 1331-56, 1994.

Montgomery, C. J., G. Kosaly, and J. J. Riley, "Direct Numerical Simulation of Turbulent Nonpremixed Combustion with Multistep Hydrogen-Oxygen Kinetics", *Comb. Flame*, Vol. 109, pp. 113-144, 1997.

Nilsen, V., and G., Kosaly, "Differentially Diffusing Scalars in Turbulence", *Phys. Fluids*, Vol. 9, pp. 3386-3397, 1997.

Nilsen, V., G. Kosaly, and J. J. Riley, "Modeling of differentially diffusing scalars in reacting turbulent flows", Western State Section of the Combustion institute, Livermore, CA, 1997.

Nilsen, V. and G. Kosaly, "Differential Diffusion in Turbulent Reacting Flows", *Comb. Flame*, Vol. 117, pp. 493-513, 1999.

Peters, N.,"Turbulent Combustion", Final Draft sent to Cambridge University Press, (1999)

Pitsch, H., and N. Peters, "A consistent flamelet formulation for non-premixed combustion considering differential diffusion effects", *Comb. Flame*, Vol. 114, pp. 26-40, 1998.

LIST OF PUBLICATIONS

Archival refereed publications

Cha,C.M., and G. Kosály, (2000) "Quasi-steady Modeling of Turbulent Nonpremixed Combustion", *Comb. Flame.* Accepted for publication.

Cook, A. W., and J. J. Riley, (1997)"Subgrid-scale modeling for turbulent reacting flows", *Comb. Flame,* Vol. 109, pp. 439-448.

Cook, A.W., J. J. Riley and G. Kosály (1997) "A Laminar Flamelet Approach to Subgrid-Scale Chemistry in Turbulent Flows," *Comb. Flame*, Vol. 109, pp.332-341.

de Bruyn Kops, S.M. and J. J. Riley, (1998) "Direct Numerical Simulation of Laboratory Experiments in Isotropic Turbulence", *Phys. Fluids,* , Vol. 10, pp. 2125-2127.

de Bruyn Kops, S.M., J. J. Riley, G. Kosály and A. W. Cook (1998) , "Investigation of modeling for non-premixed turbulent combustion", *Flow, Turb. and Comb..*
Vol. 60, pp.105-122.

de Bruyn Kops, S.M., and J. J. Riley, (2000)"Mixing Models for Large-eddy Simulation of Non-premixed Turbulent Combustion" , *Journal of Fluid Engineering,* Submitted for publication, 2000.

de Bruyn Kops, S. M. and J. J. Riley, (2000)"Re-examining the Thermal Mixing Layer with Numerical Simulations", *Phys. Fluids,* Vol. 12, pp. 185-192.

Montgomery, C. J. , G. Kosály and J.J. Riley, (1997) "Direct Numerical Simulation of Turbulent Nonpremixed Combustion with Multistep Hydrogen - Oxygen Kinetics", *Comb. Flame*, Vol.109, pp.113-144.

Nilsen,V., and G. Kosály, (1997) "Differentially Diffusing Scalars in Turbulence", *Phys. Fluids,* Vol. 9, p.3386.

Nilsen,V., and G. Kosály, (1999) "Differential Diffusion in Reacting Turbulence", *Comb. Flame,* Vol. 117, pp. 493-513.

Presentations

J. J. Riley. 1997. Invited presentation at the Workshop on Turbulent Transport and Modeling, Los Alamos National Laboratory, June.

J. J. Riley and A. W. Cook. 1997. Invited presentation at the conference Computing the Future II; Computational Fluid Dynamics and Transonic Flow, June. This paper was subsequently published as: Cook, A. W., and J. J. Riley. 1998. Progress in subgrid-scale combustion modeling, in *Computational Fluid Dynamics Review 1997*, M. Hafez, ed., Wiley.

J. J. Riley. 1997. Invited seminar at the Battelle Pacific Northwest National Laboratory, August.

J. J. Riley, G. Kosály, and A. W. Cook. 1997. Invited presentation at the Combustion Modeling Workshop, Sandia National Laboratory, August.

Nilsen, V. and Kosály, G., 1997 "Differentially Diffusing Scalars in DNS Turbulence," AIAA 35th Aerospace Sciences Meeting & Exhibit, Reno, Nevada, January 6-10, 1997, Paper No. 97-0256

Nilsen, V., G. Kosaly, and Riley, J. J., 1997 "Modeling of Differentially Diffusing Scalars in Reacting Turbulent Flows," Western State Section of the Combustion Institute, Livermore, California, April 14-15, 1997, Paper 97S-052

Nilsen, V., 1997 "Modeling of Differentially Diffusing Scalars in Reacting Turbulent Flows," invited speaker at the Center for Turbulence Research, Stanford, California, April 18, 1997

deBruynKops, S. M., Kosály, G., and Riley, J. J., 1997 "LES of Turbulent Diffusion Flames," Poster presented at the meting of the International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames, June 3-4, 1997, Heppenheim, Germany.

Kosály, G., and Riley, J. J., 1997 "Evaluation of Closure Models of Turbulent Diffusion Flames," ARO/AFOSR Contractors Meeting in Chemical Propulsion, Ohio Aerospace Institute, June 17-19.

Nilsen, V., 1997 "Differentially Diffusing Scalars in DNS Turbulence," invited speaker at Sandia National Laboratories, Livermore, California, June 24.

deBruynKops, S. M., Kosály, G., and Riley, J. J., 1997 "Large Eddy Simulations of Non-premixed Turbulent Reacting Flows," 50th Annual meeting of the DFD, APS, San Francisco, CA, November 23--25.

V. Nilsen, W. E. Mell, and G. Kosály, 1997 "On Reynolds Number Similarity in Turbulent Flows," 50th Annual meeting of the DFD, APS, San Francisco, CA, November 23-25.

J. J. Riley. 1998. Invited lectures at the Second ERCOFTAC Summer School, Stockholm, Sweden, June. These lectures were subsequently published as: Riley, J. J. 1999. *Turbulent Combustion Modeling, in Transition, Turbulence and Combustion Modeling*, A. Hanifi et al., eds., Kluwer.

J. J. Riley. 1998. Invited seminar at Lawrence Livermore National Laboratory, July.

J. J. Riley. 1998. Invited seminar at Stanford University, July.

J. J. Riley. 1998. Invited seminar at the Annual Meeting of the Mexican Physical Society, San Luis Petosi, Mexico, November.

G. Kosály: 1998. "Recent Developments in the Modeling of Diffusion Flames," Center for Turbulent Research, Stanford University Feb.~(1998)

Chong Cha, G. Kosály, and J.C. Kramlich, 1998 "Quasi-Steady Modeling in a Hydrogen/Air Jet," Third International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames, Boulder CO, July 30--Aug 1.

V.Nilsen and G.Kosály, 1998 "Differential diffusion in turbulent reacting flows," Third International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames, Boulder CO, July 30--Aug 1.

V. Nilsen and G. Kosály, 1998 "Differential Diffusion in Turbulent Reacting Flows," at American Physical Society Division of Fluid Mechanics Annual Meeting, Philadelphia, PA, 22-25 Nov.

J. J. Riley. 1999. Invited seminar at the California Institute of Technology, January.

J. J. Riley. 1999. Invited presentation at the Second AFOSR Conference on DNS and LES, Rutgers University, June.

S. M. de Bruyn Kops and J. J. Riley. 1999. Invited seminar at Lawrence Livermore National Laboratories, July.

J. J. Riley. 1999. Invited presentation at the Workshop on Turbulence Measurements for LES, sponsored by NSF, AFOSR, ONR, DARPA and DOE, October.

J. J. Riley and S. M. de Bruyn Kops. 1999. Presentation at the Annual Meeting of the Division of Fluid Dynamics of the American Physical Society, New Orleans, November.

G.Kosály,1999 "Quasi-Steady Approximation in Diffusion Flame Modeling" at University of California, San Diego, March.

G.Kosály,1999 "Differential Diffusion in Reacting Flows" at Center For Turbulence Research, Stanford University, February.

PERSONNEL

Faculty: G. Kosály (Co-PI), J. J. Riley (Co-PI).
PhD students: S. M. deBruynKops (graduated in 1999), V. Nilsen (graduated in 1998), Y. Zhu (ongoing), P. Sripakagorn (ongoing). S. Mitarai (ongoing).
MSc students: D. Yong (Applied Math), C. Flynn (graduated in 1998).

SIGNIFICANT INTERACTIONS

J. J. Riley was co-organizer of the Workshop on Turbulence Measurements for LES, sponsored by NSF, AFOSR, ONR, DARPA and DOE, October, 1999. The report resulting from the workshop, co-authored by Riley, is available on the WWW at: http://www.me.washington.edu/les/.